CHEMFLUX™

2D / 3D Contaminant Transport Modeling Software

Tutorial Manual

Written by:
Robert Thode, B.Sc.G.E.

Edited by:
Murray Fredlund, Ph.D.

SoilVision Systems Ltd.
Saskatoon, Saskatchewan, Canada

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1 ChemFlux Tutorial Manual 4
1.1 Introduction 6
1.2 Sudicky Model 6
1.2.1 Steady-State SVFLUX Model 6
1.2.2 CHEMFLUX Model 13
1.2.3 Appendix A 22
1.3 References 23
1.4 A Three-Dimensional Example Model 24
1.4.1 Steady-State SVFLUX Solution 24
1.4.2 Appendix B 39

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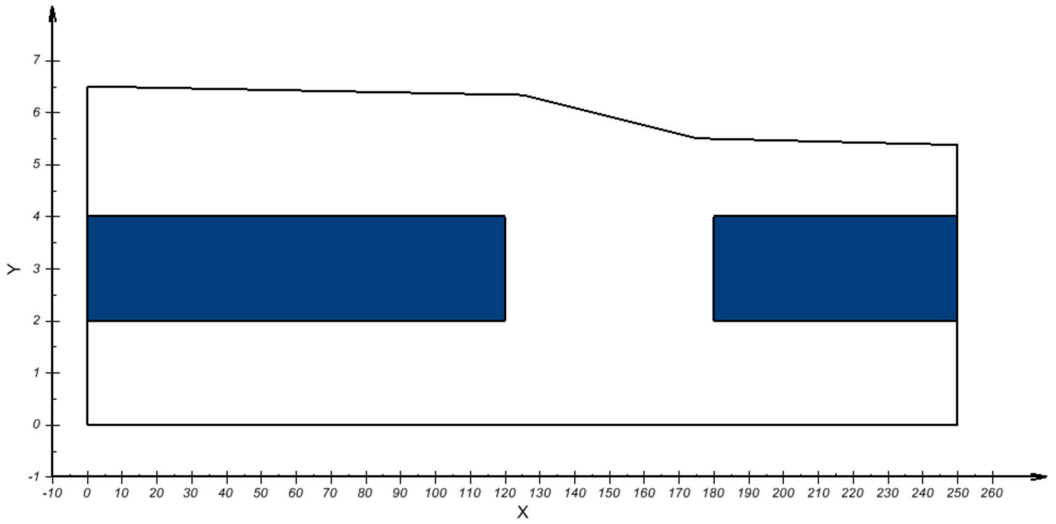
1.1 Introduction

The Tutorial Manual serves a special role in guiding the first time users of the CHEMFLUX software through a typical example problem. The example is "typical" in the sense that it is not too rigorous on one hand and not too simple on the other hand.

The Tutorial Manual serves as a guide by: assisting the user with the input of data necessary to solve the boundary value problem, ii.) explaining the relevance of the solution from an engineering standpoint, and iii.) assisting with the visualization of the computer output. An attempt has been made to ascertain and respond to questions most likely to be asked by first time users of CHEMFLUX.

1.2 Sudicky Model

Sudicky (1989) developed the following example. The model considers flow and solute transport in a heterogeneous cross section with a highly irregular flow field, dispersion parameters that are small compared with the spatial discretization, and a large contrast between longitudinal and transverse dispersivities (Zheng and Wang, 1999).



It is important to note that you will be analyzing the SVFLUX model before the CHEMFLUX model is completed.

1.2.1 Steady-State SVFLUX Model

The completed model is present under the project and model listed below. The user may open this model to run and display the results of the analysis. The user can also recreate this model under a separate model file.

Project:	ContaminantPlumes
Model:	VanderHeijdeSS, VanderHeijde
Minimum authorization required:	FULL

The seepage model shown below gives the model dimensions, boundary conditions, material properties, and the final flow regime. This is followed by step by step instructions on how to enter and solve the contaminant

transport model.

Model Description

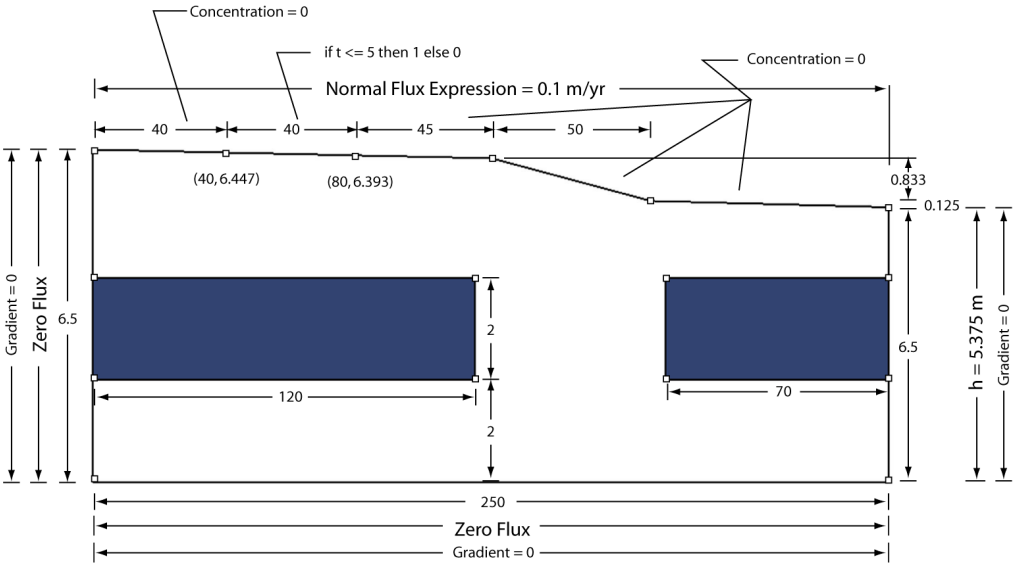


Figure 1 - 2D example, model dimensions

Material Properties

Material Properties used for the SVFLUX steady-state model are as follows:

k_{sat} = 158 m/yr
k_y-ratio = 1.0
Volumetric water content = 0.35

k_{sat} = 3156 m/yr
k_y-ratio = 1.0
Volumetric water content = 0.35

The soil-water characteristic curve data was used for both materials in the model.

Table 1

Soil Suction (kPa)	Volumetric Water Content Ratio
0.0001	0.351
100	0.35
1000	0.349

NOTE:

Steady-state seepage solutions do not require that the soil-water characteristic curves have an initial positive slope. An initial positive slope is only required in transient models where water storage will change with time. The initial positive slope on the SWCC applies for the low suction range.

- **SVFLUX Flow Regime**

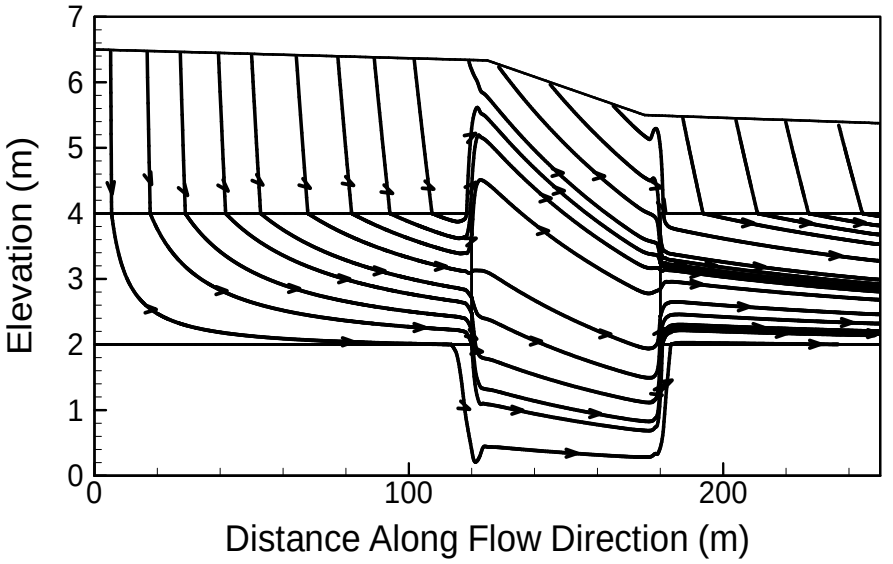


Figure 2 - 2D example, flow regime

1.2.1.1 Model Setup

In order to set up the model described in the preceding section, the following steps (or categories) will be required:

a. Create model
b. Enter geometry
c. Specify boundary conditions
d. Apply material properties
e. Specify model output
f. Run model
g. Visualize results

a. Create Model

Since FULL authorization is required for this tutorial, the user must perform the following steps to ensure full authorization is activated:

1. Plug in the USB security key,
2. Go to the File > Authorization dialog on the SVOFFICE Manager.
3. Software should display full authorization of Standard or Professional. If not, it means that the security codes provided by SoilVision Systems at the time of purchase have not yet been

entered. Please see the the Authorization section of the SVOFFICE User's Manual for instructions on entering these codes.

The following steps are required to create the model:

1. Open the SVOFFICE Manager dialog.
2. Select "ALL" under the Applications combo box and "ALL" for the Model Origin combo box.
3. Create a new project called *UserTutorial* by pressing the *New* button next to the list of projects.
4. Create a new model called *User_Vanderheijde* by pressing the *New* button next to the list of models. The new model will be automatically added under the recently created *UserTutorial* project. Use the settings below when creating a new model.
5. Select the following:
   - *SVFlux* for Application
   - *2D* for System,
   - *Steady-State* for Type,
   - *Metric* for Units, and
   - *Seconds (s)* for Time Units.

   Click on OK.

Before entering any model geometry it is best to set the World Coordinate System to ensure that the model will fit into the drawing space.

1. Access the World Coordinate System tab by selecting the *World Coordinate System* tab on the Create New Model dialog.
2. Enter the *World Coordinates System* coordinates shown below into the dialog.

   x-minimum = -10
   y-minimum = -2
   x-maximum = 260
   y-maximum = 8

3. Click *OK* to close the dialog.

For better viewing results, set the magnification factor in the View Settings:

1. Select View > Settings from the menu.
2. Set the aspect ratio near 1:10. This will magnify the model's height.
3. Click *OK* to close the dialog.

b. Enter Geometry

The geometry must be defined for the SVFLUX model.

1. Add *Region:* The model is created with one default region. Another region can be added under the *Model > Geometry > Regions dialog* by pressing the *New* button and closing the dialog.
2. Select *Region:* The user must select the region they would like to draw using the Draw > Region Polygon from the menu.
3. Draw *Region 1:* The first region can be extended by drawing the geometry on the CAD window using the *Draw > Region Polygon* command. Alternatively, the *Region Properties* dialog can be opened (*Model > Geometry > Region Properties*) and the region polyline points cut and pasted in from the provided spreadsheet. The points can also be pasted into the dialog. See Appendix A for the geometry of each region.
4. Select *Region 2:* The user must select Region 2 as the current region on which to draw.
5. Draw *Region 2:* The second region can be entered in a manner similar to that explained for Region 1.
6. Repeat for Region 3.

c. Specify Boundary Conditions

Flow models must generally have a defined entry and exit point for water to flow. The boundary conditions shown at the start of this model can be entered using the following steps:

1. Select *Region 1*: Region 1 must be selected by clicking on the region.
2. Enter *Boundary Conditions #1*: The *Boundary Conditions* dialog can be displayed under the *Model > Boundary Conditions > Properties* menu option. Once in the dialog the user needs to:
   - select the *node point, (250, 5.375),*
   - then select a normal flux expression from the combo box,
   - enter a value of *0.1* m/yr.
   - select the *point (0, 6.5),* and
   - select the *Zero Flux* expression from the boundary condition drop-down box.
3. Enter *Boundary Condition #2:* The node (250,0) must be selected in the *Boundary Conditions* dialog. The user must then:
   - select a Head Expression boundary condition type, and
   - enter a value of 5.375 m.
4. Close the dialog. The newly specified boundary condition will be displayed with symbols on the CAD window.

A summary of the boundary conditions for this model can be found in Appendix A.

d. Apply Material Properties

Material Properties must now be entered and applied to specific regions in the model. The following steps are required in order to properly apply material properties:

1. Open Materials Manager: *Model > Material > Manager*.
2. Click *New*: This will open a new material record. Enter *ChemFlux Soil1* as the material name and click OK.
3. Enter *Properties*: The material properties for ChemFlux Soil1 must be entered. Click the *Properties* button on the Material Manager dialog.
4. Laboratory SWCC data: Choose the SWCC tab and click the *Data* button. Enter the material properties as found in Table 1. Click OK to accept the data entered and close the SWCC Data dialog.
5. Fitting: Laboratory data can be best fit with the Fredlund & Xing (1994) soil-water characteristic curve equation. Fitting the curve can be accomplished through the following steps:
   a. Select *Fredlund & Xing* as the fitting method from the SWCC drop-down.
   b. Enter *0.351* in the field for Saturated VWC.
   c. Click the *Properties* button to set the properties of the Fredlund & Xing fit.
   d. Click the *Apply Fit* button.
6. Enter the Hydraulic Conductivity data: Choose the Hydraulic Conductivity Tab and enter the K_{sat} and *Ky-ratio* values. The dialog can be closed once material properties are entered. The ChemFlux Soil2 material's properties are available in Appendix A and can be entered in the same manner as ChemFlux Soil1.
7. Apply to regions: The material properties can be applied to regions by opening the Regions dialog *(Model > Geometry > Regions)* and selecting the appropriate materials from the drop-down boxes. ChemFlux Soil1 should be applied to Region 1 and ChemFlux Soil2 should be applied to Regions 2 and 3.

e. Specify Model Output

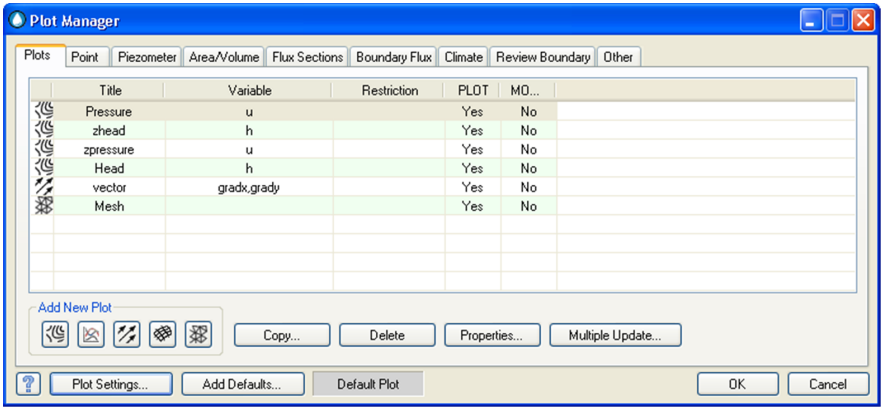
Two levels of output may be specified: i) output (graphs, contour plots, fluxes, etc.) which are displayed during model solution, and ii) output which is written to a standard finite element file for viewing with AcuMesh software. Output is specified in the following two dialogs in the software:

i) Plot Manager:	Output displayed during model solution.
ii) Output Manager:	Standard finite element files written out for visualization in AcuMesh or for initial condition input to other finite element packages.

PLOTMANAGER

The plot manager dialog is first opened to display appropriate solver graphs. There are many plot types that can be specified to visualize the results of the model. A few will be generated for this tutorial example model, including a plot of the solution mesh, pressure contours, head contours, and gradient vectors.

1. Open the Plot Manager dialog by selecting *Model* > *Reporting* > *Plot Manager* from the menu.



2. The toolbar at the bottom left of the dialog contains a button for each plot type. Click on the *Contour* button to begin adding the first contour plot. The Plot Properties dialog will open.
3. Enter the title *'Pressure'*.
4. Select *'u'* as the variable to plot from the drop-down.
5. Click the Output Options tab and ensure that only *Plot* is checked off.
6. Click *OK* to close the dialog and add the plot to the list.
7. Repeat steps 2 to 6 to create the plots shown in the above dialog. The zoomed plots are not necessary, they are used to closely examine key zones in the problem.
8. Click *OK* to close the Plot Manager and return to the workspace.

Alternatively, the user may press the *Add Default Plots* button and typical plots will be added to the plot list.

OUTPUTFILES

There are four output file types that can be specified to export the results of the model. One will be generated for this tutorial example model: a plot to transfer the results to ACUMESH.

1. Open the Output Manager dialog by selecting *Model* > *Reporting* > *Output Manager* from the menu.
2. The toolbar at the bottom left corner of the dialog contains a button for each output file type. Click on the *ACUMESH* button to add the output file with the default variables.
3. Press the *CHEMFLUX* button to add the output file with the default variables.

4. Click *OK* to close the dialog and add the output file to the list.
5. Click the *Settings* button on the Output Manager dialog to open the Output Settings dialog.
6. Ensure the Region Separation checkbox is checked; press *OK* to close the dialog.
7. Click *OK* to close the Output Manager and return to the workspace.

f. Run Model

The current model can be run by selecting the *Solve > Analyze* menu option.

g. Visualize Results

The flow vectors for the current model can be visualized through the following steps:

1. Open *ACUMESH: View > ACUMESH* menu option
2. *Plot Flow Lines: Plot > Flow Lines*

1.2.1.2 Results and Discussion

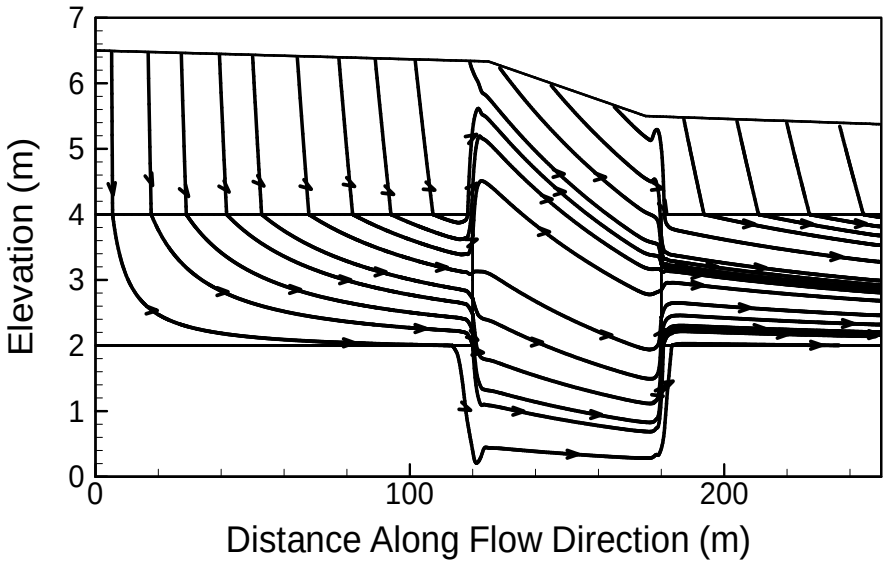


Figure 3 ACUMESH flowlines for steady-state flow regime.

1.2.2 CHEMFLUX Model

Now that the steady-state flow hydraulic head gradients have been established in the SVFLUX software the focus turns to solving for the chemical concentrations with time for the solution domain. In order to solve this model the user needs to perform the following steps:

1. Create a new CHEMFLUX model,
2. Apply appropriate boundary conditions in the CHEMFLUX model, and
3. Apply appropriate material properties.

The methodology for setting up the model is detailed in the following sections.

Model Description

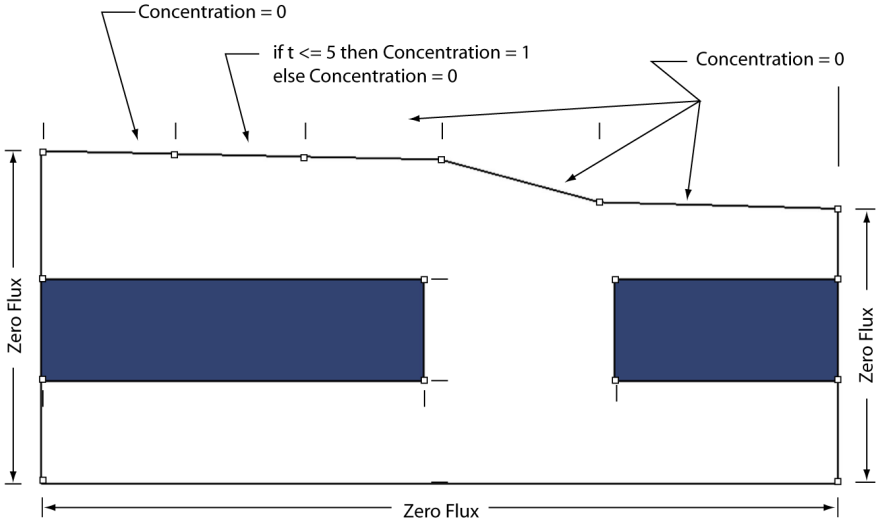


Figure 4 - The 2D Vanderheijde example, showing boundary conditions for the CHEMFLUX model

Material Properties

The material properties for the numerical model are as follows:

Longitudinal Dispersivity, α_L = 0.5m
Transverse Dispersivity, α_T = 0.005m
Diffusion Coefficient, D^* = 0.0423m^2/yr

1.2.2.1 Model Setup

In order to set up the model described in the preceding section, the following steps are required. The steps fall under the general categories of:

a. Create model
b. Enter geometry
c. Specify boundary conditions
d. Apply material properties
e. Specify model output
f. Run model

g. Visualize results

a. Create Model

A gradient file generated by SVFLUX is required for this example. The seepage model described above has been included in the model files distributed with the SVFLUX software. This file was generated previously in the Steady-State SVFLUX model example.

When the solution for the model is finished, a gradient file will be automatically created in the solution folder by SVFLUX. The file is called *gradient.trn.*

The user must decide the project under which the CHEMFLUX model is going to be organized. If the project is not yet included in the Projects section of the SVOFFICE Manager, you must add the project before proceeding with creating the model. In this case, the model is placed under the project called UserTutorial. To add a model:

1. Open the SVOFFICE Manager dialog.
2. Select the project called *UserTutorial.*
3. Press the *New* button under the *Models* heading.
4. Select *CHEMFLUX* for the Application.
5. Enter *User_Example2D* in the Model Name box.
6. Select *2D* for System, *Transient* for Type, Metric for Units, and Years for Time Units.
7. Click the *OK* button to save the model and close the New Model dialog.
8. The new model will automatically added be added to the Models list.

NOTE:
You will notice that there is no distinction between steady-state and transient state in CHEMFLUX. This is because all CHEMFLUX models are considered to be transient state.

b. Enter Geometry

The geometry for the model can be obtained in the spreadsheet located here. Entering the geometry into the newly created SVFLUX model can be accomplished through the following steps:

1. Select the *Model* > *Geometry* > *Import Geometry* > *From Existing Model...* menu.
2. The Import Geometries dialog will pop up. Select the appropriate project name, *Tutorial.*
3. Select the *Vanderhiejde* model.
4. Press the *Import* button.

The World Coordinate Settings and the View Settings may need to be set up again:

1. Access the World Coordinate System dialog by selecting View > *World Coordinate System* from

the menu.

2. Enter the *World Coordinates System* coordinates shown below into the dialog.

   x-minimum = -10
   y-minimum = -2
   x-maximum = 260
   y-maximum = 8

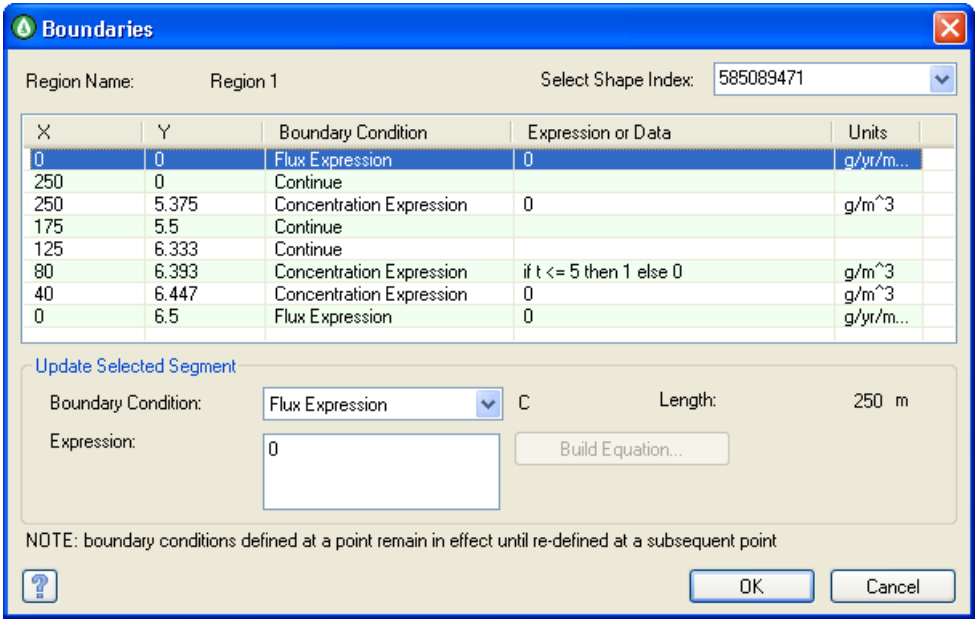
3. Click *OK* to close the dialog.

For better viewing results, set the magnification factor in the View Settings:

1. Select View > Settings from the menu.
2. Set the aspect ratio near 1:10. This will magnify the model's height.
3. Click *OK* to close the dialog.

c. Specify Boundary Conditions

In general, flow models must have a defined entry and exit point for water to flow. The boundary conditions shown at the start of this model may be entered through the following steps:


Boundaries
Region Name: Region 1
Select Shape Index: 585089471
X Y Boundary Condition Expression or Data Units
0 0 Flux Expression 0 g/yr/m...
250 0 Continue
250 5.375 Concentration Expression 0 g/m^3
175 5.5 Continue
125 6.333 Continue
80 6.393 Concentration Expression if t <= 5 then 1 else 0 g/m^3
40 6.447 Concentration Expression 0 g/m^3
0 6.5 Flux Expression 0 g/yr/m...
Update Selected Segment
Boundary Condition: Flux Expression C Length: 250 m
Expression: 0
Build Equation...
NOTE: boundary conditions defined at a point remain in effect until re-defined at a subsequent point
OK
Cancel

1. *Select Region 1*: Region 1 must be selected by clicking on the region.
2. *Enter Boundary Conditions*: The *Boundary Conditions* dialog may be displayed under the *Model > Boundary Conditions > Properties* menu option. Once in the dialog the user needs to:
   - Select the *point* (0,0) from the list,

- From the *Boundary Condition* drop-down select a *Flux Expression* boundary condition equal to 0,
- Repeat these steps to define the boundary conditions for the remaining Region 1 segment as shown in the diagram and in the screen-shot above. (Be sure to define a *Flux Expression* boundary condition equal to 0 for the last point in the list).

3. Close the dialog. The newly specified boundary condition will be displayed with symbols on the CAD window.

d. Apply Material Properties

Material Properties must now be entered and applied to specific regions in the model. The following steps are required in order to properly apply material properties:

1. Open *Materials Manager: Model > Material > Manager*.
2. Click *New:* This will open a new material record.
3. Enter *Properties:* Move to the *Dispersion* tab. Enter the Longitudinal Dispersivity, α_L = 0.5 m. Enter the Transverse Dispersivity, α_T = 0.005 m. Select Constant as the Diffusion option. Enter the Diffusion Coefficient, D^* = 0.0423 m^2/yr.
4. Apply to regions:
   - Open the regions dialog selecting *Model > Geometry > Regions* from the menu.
   - Select *Material#1* from the drop-down as the material for Region 1.
   - Repeat for Region 2 and Region 3.
   - Click *OK* to close the dialog.

Next, the settings that will be used for the model must be specified. To open the *Settings* dialog select *Model > Settings* in the workspace menu.

The *Settings* dialog will contain information about the current model *System, Units, Time*, and contaminant transport processes.

1. To open the Settings dialog select *Model > Settings* in the workspace menu.
2. Check *Advection* and *Dispersion* in the Processes box under the General tab.
3. Choose the *Time* tab. Enter a Start Time of 0, a Time Increment of 1 yr, and an End Time of 20 yr.
4. Select the *Advection* tab.
5. Choose *Import* from the Advection Control option.
6. Click *Browse*.
7. Specify the gradient file *Examples_ChemFlux2D.trn* that was generated by SVFLUX in the

previous example.

8. Press *OK* to close the Settings dialog.

NOTE:

It is very important that the .TRN file and the geometry are obtained from the same SVFLUX model.

e. Specify Model Output

Two levels of output may be specified: i) output (graphs, contour plots, fluxes, etc.) which are displayed during model solution, and ii) output which is written to a standard finite element file for viewing with AcuMesh software. Output is specified in the following two dialogs in the software:

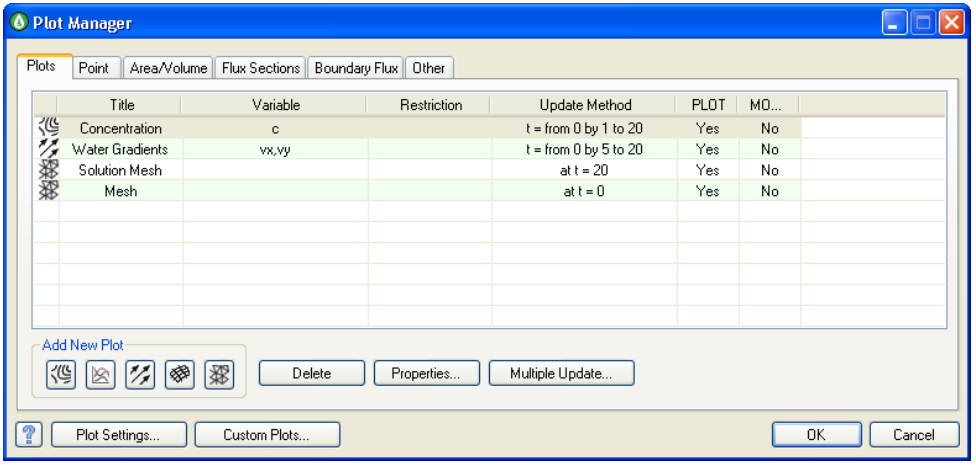
i) Plot Manager: Output displayed during model solution.

ii) Output Manager: Standard finite element files written out for visualization in AcuMesh or for inputting to other finite element packages.

PLOTMANAGER

The plot manager dialog is first opened to display appropriate solver graphs. The next step in model setup is to specify the data which will be generated by the finite element solver. Both the graphs displayed by the FlexPDE solver as well as the output generated for the subsequent CHEMFLUX analyses must be specified.

1. Open the Plot Manager dialog by selecting *Model* > *Reporting* > *Plot Manager* from the menu.
2. The toolbar at the bottom left corner of the dialog contains a button for each plot type. Click on the *Contour* button to begin adding the first contour plot. The Plot Properties dialog will open.
3. Enter the title *Concentration.*
4. Select *c* as the variable to plot from the drop-down.
5. Select the *PLOT* from the Output Option tab.
6. Move to the *Update Method* tab and enter a Start Time = 0, a Time Increment = 1, and an End Time = 20.
7. Move to the *Zoom* tab and enter *X* = 100, *Y* = 0.1, Width = 100, and Height = 6.6.
8. Click *OK* to close the dialog and add the plot to the list.
9. Repeat steps 2 to 8 to create the remaining plots. Note that the Mesh plot does not require entry of a variable.
10. Click *OK* to close the Plot Manager and return to the workspace.



OUTPUTMANAGER

There are many output file types that can be specified to export the results of the model. One will be generated for this tutorial example model: a file to transfer the results to ACUMESH.

1. Open the Output Manager dialog by selecting *Model* > *Reporting* > *Output Manager* from the menu.

2. The toolbar at the bottom left corner of the dialog contains a button for each output file type. Click on the *ACUMESH* button to begin adding the output file. The Output File Properties dialog will open.
3. Enter the title *ACUMESH*.
4. Click *OK* to close the dialog and add the output file to the list.

Specify Time Steps:
The Output File Properties dialog also allows the user to define timesteps for the current model. This can be accessed by using the Update Method tab on the Output File Properties dialog.

1. Enter a Start Time of *0*, a Time Increment of 1 yr, and an End Time of 20 yr.
2. Click *OK* to close the Output File Properties dialog and return to the workspace.
3. Click *OK* to close the Output Manager and return to the workspace.

f. Run Model

The current model may be run by selecting the *Solve* > *Analyze* menu option.

g. Visualize Results

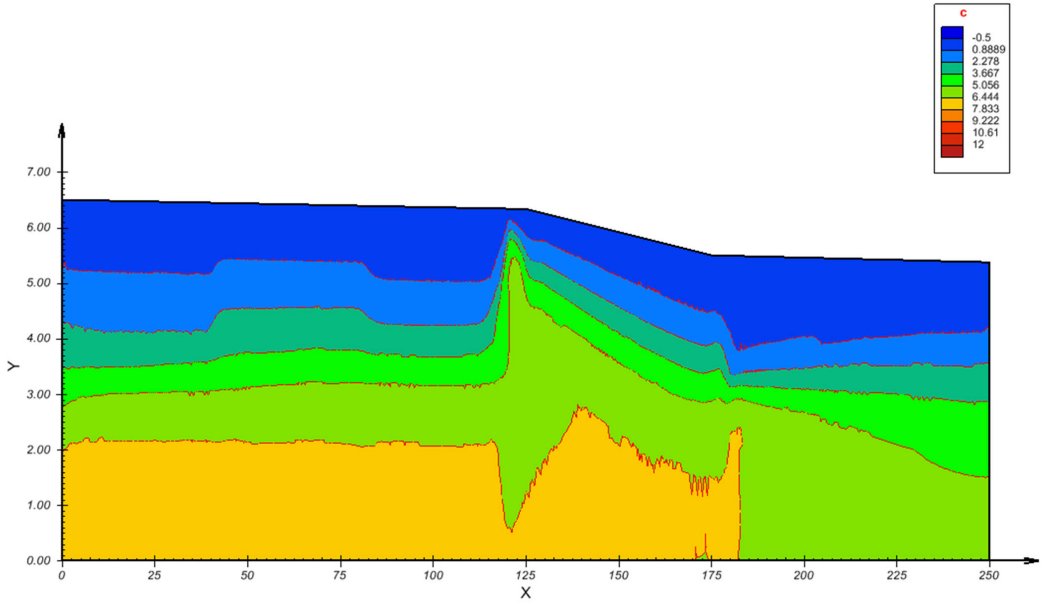
The flow vectors for the current model may be visualized through the following steps:

1. Open *ACUMESH*: *View* > *ACUMESH* menu option.

1.2.2.2 Results and Discussion

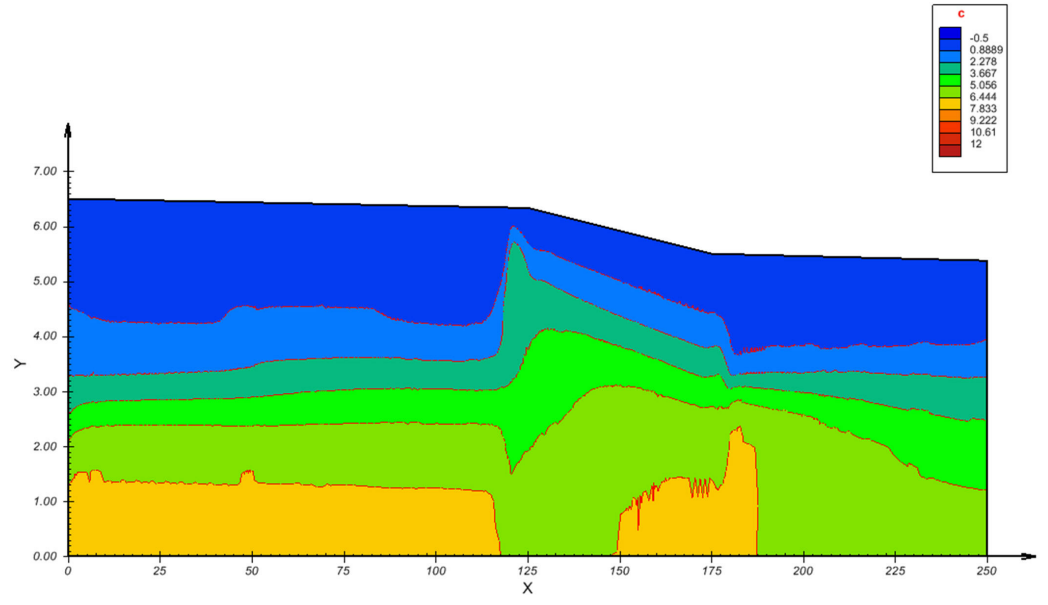
After the model has finished solving, the results will be displayed in the dialog of thumbnail plots within the CHEMFLUX solver. Right-click the mouse and select *Maximize* to enlarge any of the thumbnail plots. The following is a short summary of plots illustrating the movement of the plume through the model for times of 8 years, 12 years, and 20 years.

- **Time = 8 years**

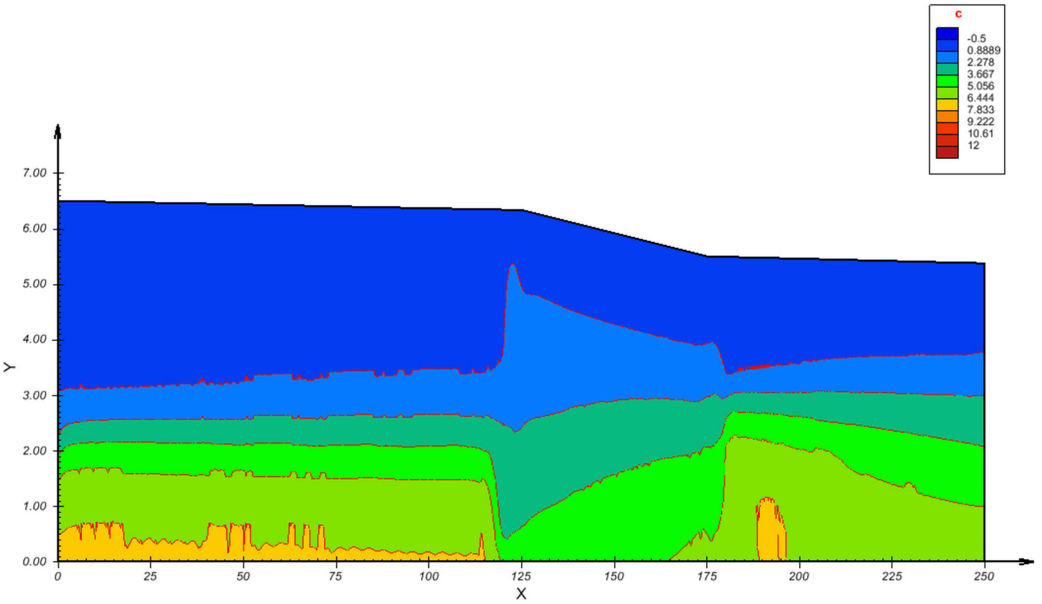


The source has been shut off for 3 years

- **Time = 12 years**



- **Time = 20 years**



1.2.3 Appendix A

Region 1

X	Y
0	0
250	0
250	5.375
175	5.5
125	6.333
80	6.393
40	6.447
0	6.5

Region 2

X	Y
0	2
120	2
120	4
0	4

Region 3

X	Y
180	2
250	2
250	4
180	4

Boundary Conditions

X	Y	Boundary Condition
0	0	Gradient Expresion = 0
250	0	Continue
250	5.375	Concentration Expression = 0
175	5.5	Continue
125	6.333	Continue
80	6.393	Concentration Expression = if t <= 5 then 1 else 0.
40	6.447	Concentration Expression = 0
0	6.5	Gradient Expresion = 0

1.3 References

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C.W. Fetter, 1993. Contaminant Hydrogeology. MacMillan Publishing Company. New York, New York.

D. G. Fredlund and H. Rahardjo, 1993. Soil Mechanics for Unsaturated Soils. John Wiley & Sons, New York

FlexPDE 3.x Reference Manual, 1999. PDE Solutions Inc. Antioch, CA 94509

Jacob Bear, 1972. Dynamics of Fluids in Porous Media. Dover Publications Inc., New York

Jacob Bear, 1979. Hydraulics of Groundwater. McGraw-Hill, New York.

Jason S. Pentland, 2000. Use of a General Partial Differential Equation Solver for Solution of Heat and Mass Transfer Problems in Soils. University of Saskatchewan, Canada

Nguyen Thi Minh Thieu, 1999. Solution of Saturated/Unsaturated Seepage Problems Using a General Partial Differential Equation Solver. University of Saskatchewan, Canada

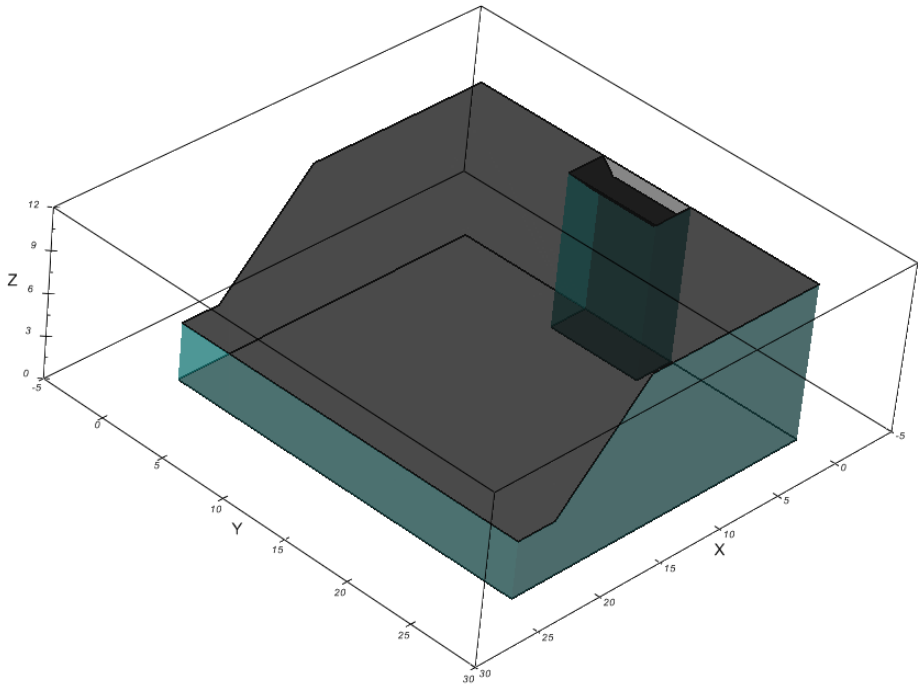
R. Allan Freeze and John A. Cherry, 1979. Groundwater. Prentice –Hall, Inc., Englewood Cliffs, New Jersey

Tecplot User's Manual, version 8.0, 1999. Amtec Engineering Inc. Bellevue, WA 98009-3633

1.4 A Three-Dimensional Example Model

The following example will introduce you to the three-dimensional model in CHEMFLUX. The model will be used to investigate if contaminant from a reservoir will travel to a river channel due to advection and dispersion processes within a 400 day time period. The 400 day time period was chosen as the time necessary to install a pumping well between the river channel and the reservoir. The well will be used to pump contaminant from the ground to ensure the plume will not reach the river channel. The example model begins with a brief description of the steady-state seepage analysis completed to provide CHEMFLUX with computed seepage gradients. Next a detailed set of instructions guides the user through the creation of the 3D contaminant transport model.

Project:	Tutorial
Model:	Example3D
Minimum authorization required:	FULL



It is important to note that you will be analyzing the SVFLUX model before the CHEMFLUX model is completed.

1.4.1 Steady-State SVFLUX Solution

Advection is known as the process by which solutes are transported by the bulk motion of the flowing groundwater Freeze and Cherry (1979). The bulk motion of the flowing groundwater or seepage gradients are solved using SVFLUX. SVFLUX calculates the seepage gradients and writes them to a text file. The CHEMFLUX solver then reads this text file when calculating the contaminant transport solution. Below is a description of the seepage model solved by SVFLUX.

Project: Ponds
Model: Reservoir3D

- **Model Dimensions**

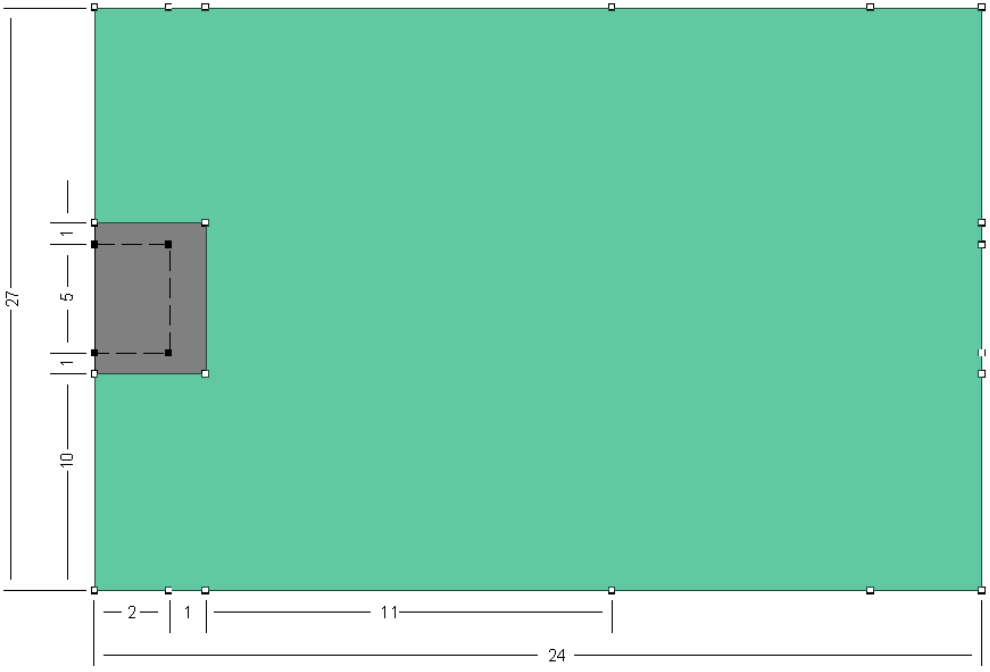


Figure 5 3D Example; Model Dimensions

The data points for the surface grids can be found Appendix B. Enter these points to set up the SVFLUX model geometry.

- **Boundary Conditions**

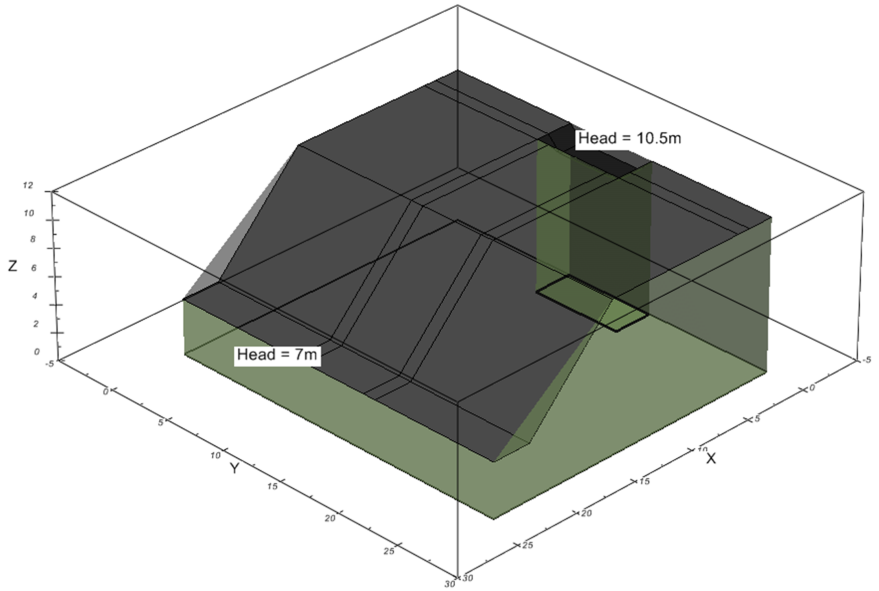


Figure 6 3D Example; Boundary Conditions

The steady-state seepage model is set up to simulate a pond or reservoir a certain distance from a river channel. The water levels in the reservoir and river channel are set using head boundary conditions. The level of water in the reservoir is set using a *Head Expression = 10.5m* set on surface 2 for the reservoir region. The level of water in the river channel is set using a *Head Expression = 7m* set on the line segment extending from point (14,0) to (14,27) on surface 1.

- **Material Properties**

There is only one material in the saturated 3D example model. Two regions have been implemented in this model in order to apply the necessary boundary conditions. The material in the model has a hydraulic conductivity, k_{sat} = 2.17e –01 m/d.

- **Flow Regime**

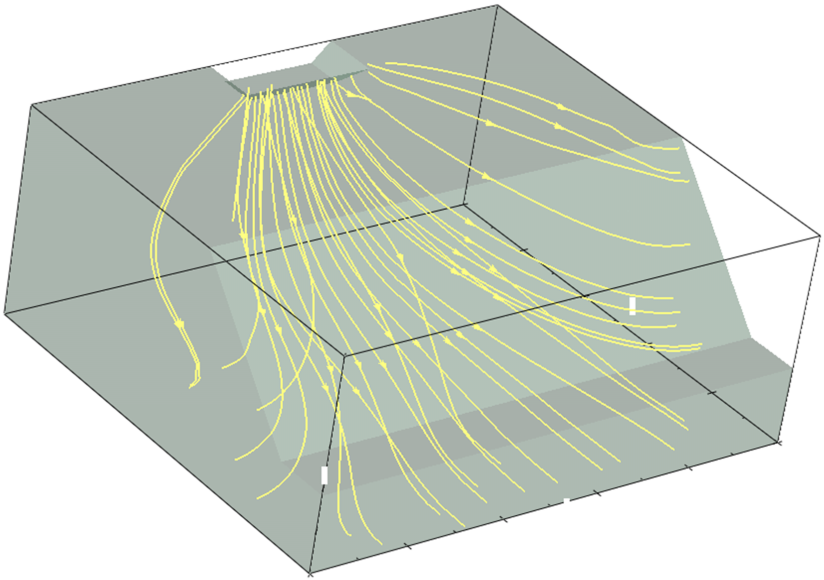


Figure 7 3D Example; Flow Regime

Flow lines show that groundwater is flowing from the reservoir toward the adjacent river channel. The presence of unsaturated material near the surface of the model is causing water to first flow down to the saturated zone and then move toward the river channel.

1.4.1.1 CHEMFLUX Model Setup

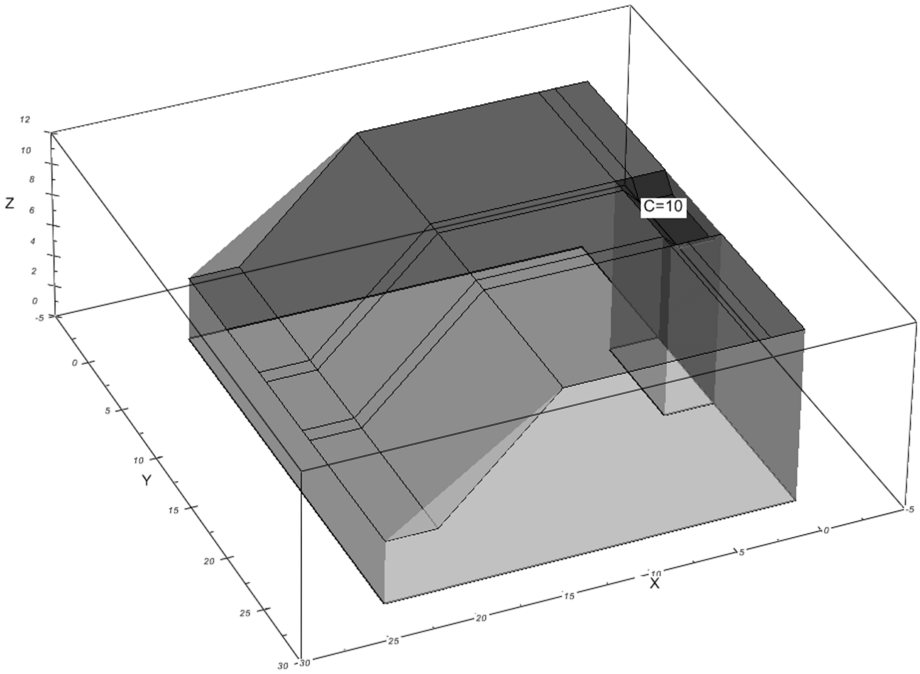


Figure 8 3D example, CHEMFLUX boundary conditions

- **CHEMFLUX Material Properties**

Please note the SVFLUX Solution shown in the diagrams above are a result of the SVFLUX Reservoir3D Tutorial. In order to set up the CHEMFLUX model described for this tutorial, the following steps will be required. The steps for creating a model fall under the general categories of:

1. Create model
2. Enter geometry
3. Specify boundary conditions
4. Apply material properties
5. Specify model output
6. Run model
7. Visualize results

1. Create Model

The first step in defining a model is to decide the project under which the model is going to be organized. If the project is not yet included you must add the project before proceeding with the model. In this case, the model

is placed under the project called Tutorial. To add a model:

1. Open the SVOFFICE Manager dialog.
2. Select the project called *UserTutorial.*
3. Press the *New* button under the *Models* heading and enter *User_CHEMFLUX3D* as the model title.
4. Select the following:
   - *CHEMFLUX* for Application
   - *3D* for System,
   - *Transient* for Type,
   - *Metric* for Units, and
   - *Days* for Time Units.
5. Click the *OK* button to save the model and close the New Model dialog.
6. The new model will automatically be opened in the workspace.

2. Enter Geometry

The geometry for the model must be imported from SVFLUX before any other modeling can be done in CHEMFLUX.

1. Select the *Model* > *Geometry* > *Import Geometry* > *From Existing Model...* menu.
2. The Import Geometries menu will pop up. Select the appropriate project name *Tutorials*.
3. Select the *Reservoir3D* model.
4. Press the *Import* button.
5. A Pop up message will appear stating *Current surfaces, geometry, features, art objects, flux sections, and plots referencing a specific region to be deleted. Do you wish to continue?* Click on *Yes.*
6. A Pop up message will appear asking if you want to copy material properties and assignments. Click on *No.*

The import includes any regions, region shapes, surfaces, surface grids and elevations. These parts of the model definition are fixed in CHEMFLUX. World coordinate system settings and features are also imported if present, but may be edited in CHEMFLUX.

3. Specify Boundary Conditions

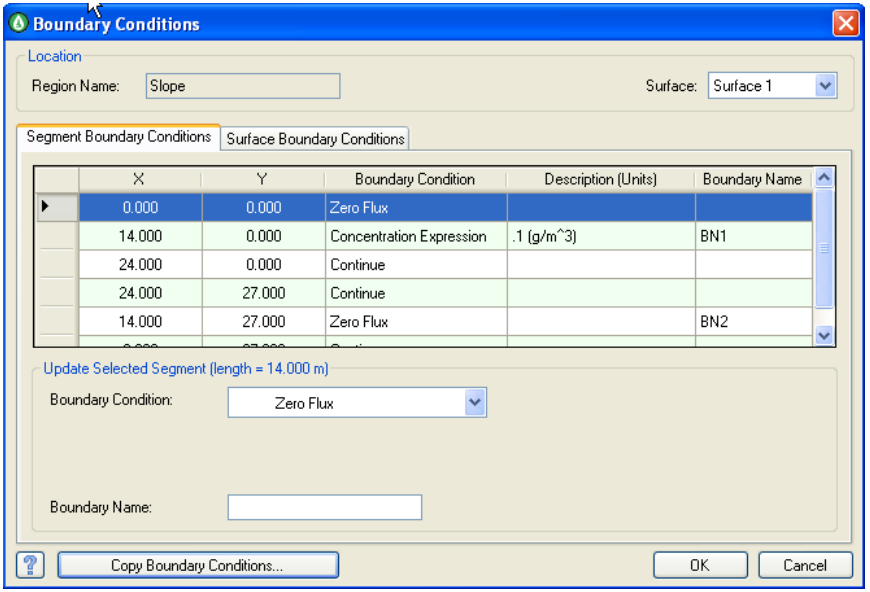
In general, flow models must have a defined entry and exit point for water to flow. The boundary conditions shown at the start of this model may be entered through the following steps:

1. Select *Region 1*: *Slope* and *Surface: 1* must be selected by clicking on the region & surface

dialogue at the top of the screen.

2. Enter *Boundary Conditions #1*: The *Boundary Conditions* dialog may be displayed under the *Model* > *Boundaries* > *Boundary Conditions* menu option. Once in the dialog the user needs to:
   - Select the starting node point, (14, 0),
   - Then select a Concentration expression from the combo box,
   - Enter a value of *0.1 g/m*^{3}.
   - Select the node point, (14, 27) and specify a zero flux boundary condition.

   Please note, although the above boundary conditions may appear to be entered already by default (from the geometry import you performed) , you still need to enter the above conditions for CHEMFLUX analysis to occur.



3. Close the dialog. The newly specified boundary condition will be displayed with symbols on the CAD window.

4. Apply Material Properties

The next step in defining the model is to specify the settings that will be used for the model.

The Settings dialog will contain information about the current model System, Units, Time, and contaminant transport processes.

1. To open the Settings dialog select *Model* > *Settings* in the menu.

2. Put a check mark in the *Advection* and *Dispersion* boxes in the Processes section under the *General* tab if they are not already there.
3. Move to the Time tab.
4. Enter a *Start Time of 0*, an Initial Increment of *50 days*, and an End Time of *400 days*.
5. Select the *Advection* tab.
6. Choose *Import* from the Advection Control option.
7. Click *Browse*.
8. Specify the file *ChemfluxInput_Reservoir3D_1.trn* that was generated by SVFLUX. This file can be found in the following directory *C:\SVS\ModelFilesSVSlope\Tutorial\3d\SteadyState \Reservoir3D*.

NOTE:
It is very important that the .TRN file and the geometry are obtained from the same SVFLUX model.

In order to improve solution time for the purposes of this tutorial certain finite-element options will be set. The finite element mesh node limit and grid spacing will be set to generate a simpler mesh that will reduce the solution time.

9. Select *Model* > *FEM Options* from the menu to open the FEM Options dialog.
10. Click on the *Advanced*>> button.
11. Click on the *Mesh Generation Controls* tab.
12. Set the *NODELIMIT* to 10000.
13. Press *OK* to close the FEM Options dialog.

The next step in defining the model is to enter the material properties for the single material that will be used in the model. Only one material is used for the model with these properties:

Longitudinal Dispersivity, α_L = 1m
Transverse Dispersivity, α_T = 1m
Diffusion Coefficient, D^* = 0m^2/day

1. Open the Materials Manager dialog by selecting *Model* > *Materials* > *Manager…* from the menu.
2. Click the *New Material* button to create a material, type in a name for the material as *3D Tutorial Soil* and click *OK*. The Material Properties dialog will open automatically.
3. Move to the *Dispersion* tab.
4. Refer to the data provided above. Enter the Longitudinal Dispersivity, α_L = 1m.

5. Enter the Transverse Dispersivity, α_T = 1m.
6. The Diffusion option is set to Constant as the gradient file specified does not contain volumetric water content, which is required to define a diffusion curve.
7. Enter the Diffusion Coefficient, D^* = 0m^2/day.
8. Close the Material Properties and Material Manager dialogs.

Each region will cut through all the layers in a model creating a separate "block" on each layer. Each block can be assigned a material or be left as *void*. A void area is essentially air space. In this model all "blocks" will be assigned a material.

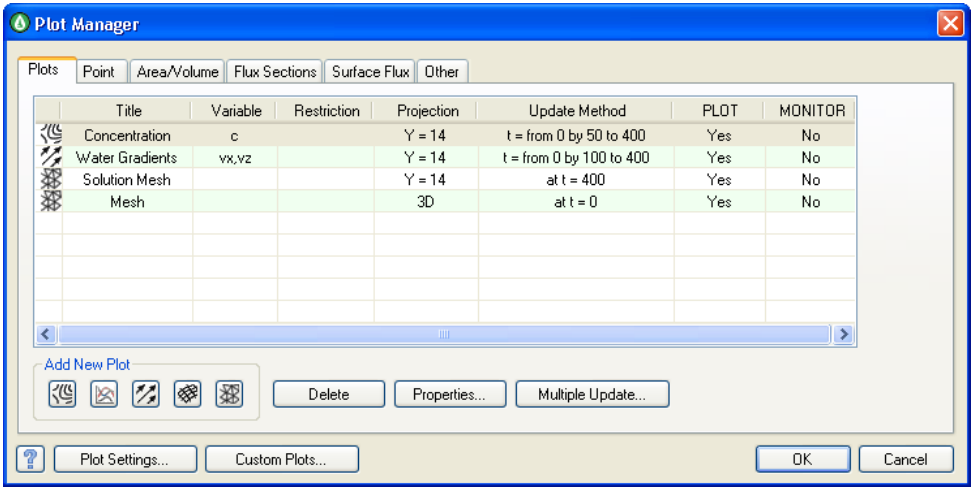
1. Select *Slope* in the Region Selector.
2. Select *Model* > *Materials* > *Region Materials* from the menu to open the Region Materials dialog.
3. Select the *3D Tutorial Soil* material from the drop-down for *Layer 1*.
4. Close the dialog using the *OK* button.
5. Select *Reservoir* in the Region Selector.
6. Select *Model* > *Materials* > *Region Materials* from the menu to open the Region Materials dialog.
7. Select the *3D Tutorial Soil* material from the drop-down for *Layer 1*.
8. Close the dialog using the *OK* button.

5. Specify Model Output

The next step is to specify the data which will be generated by the finite element solver. Both the graphs displayed by the FlexPDE solver as well as the output generated for the subsequent CHEMFLUX analysis must be specified.

There are many plot types that can be specified to visualize the results of the model. A plots few will be generated for this tutorial example model including a plot of the concentration contours, solution mesh, and water gradient vectors.

1. Open the Plot Manager dialog by selecting *Model* > *Reporting* > *Plot Manager* from the menu.



2. The toolbar at the bottom left corner of the dialog contains a button for each plot type. Click on the *Contour* button to begin adding the first contour plot. The *Plot Properties* dialog will open.
3. Enter the title *Concentration.*
4. Select *c* as the variable to plot from the drop-down.
5. Move to the *Update Method* tab.
6. If not already entered, enter in the following values for Start = 0 Increment = 50 End = 400.
7. Move to the *Projection* tab.
8. Select *Plane* Projection option.
9. Select *Y* from the Coordinate Direction drop-down.
10. Enter *14* in the Coordinate field. This will generate a 2D slice at *Y* = 14m on which the concentration contours will be plotted.
11. Move to the *Output Options* tab.
12. Select the *PLOT* output option.
13. Click *OK* to close the dialog and add the plot to the list.
14. Repeat these steps 2 to 12 to create the plots shown above. Note that the Mesh plot does not require entry of a variable under the *Description* Tab. Also note that the Solution Mesh & Mesh should only have an entry value for Start under the *Update Method* tab, Time Steps.
15. Click *OK* to close the Plot Manager and return to the workspace.

There are a few output file types that can be specified to export the results of the model. One will be generated for this tutorial example model: a file to output the results to AcuMesh for advanced visualization.

1. Open the Output Manager dialog by selecting *Model* > *Reporting* > *Plot Manager* from the menu.

2. The toolbar at the bottom left corner of the dialog contains a button for each output file type. Click on the *ACUMESH* button to begin adding the output file. The Output File Properties dialog will open.
3. The title will be entered automatically as *User_Example3D_AcuMesh*.
4. The variables *c*, *vx*, *vy*, and *vz* appear automatically as the default.
5. Type in the following values under the *Update Method*, Time Steps. Start = 0 Increment = 40 End = 400.
6. Click *OK* to close the dialog and add the output file to the list.
7. Click *OK* to close the Output Manager and return to the workspace.

6. Run Model

The current model may be run by selecting the *Solve* > *Analyze* menu option.

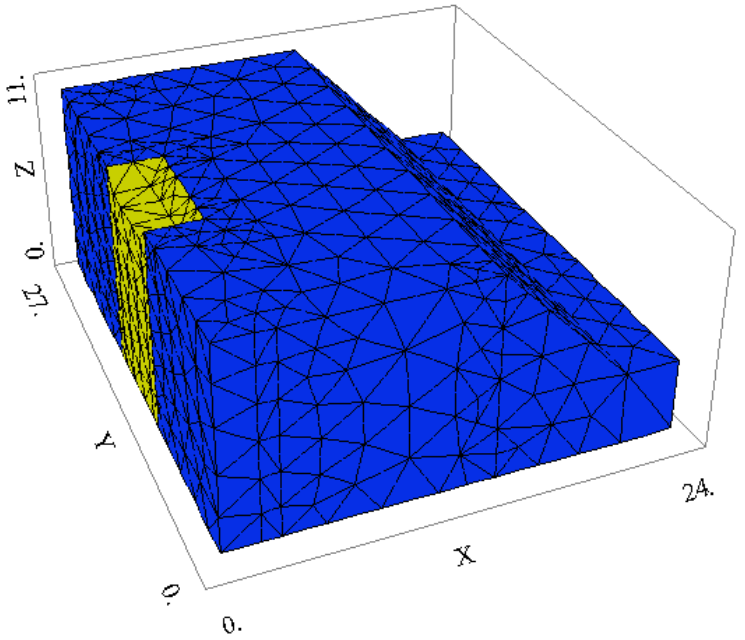
7. Visualize Results

The flow vectors for the current model may be visualized through the following steps:

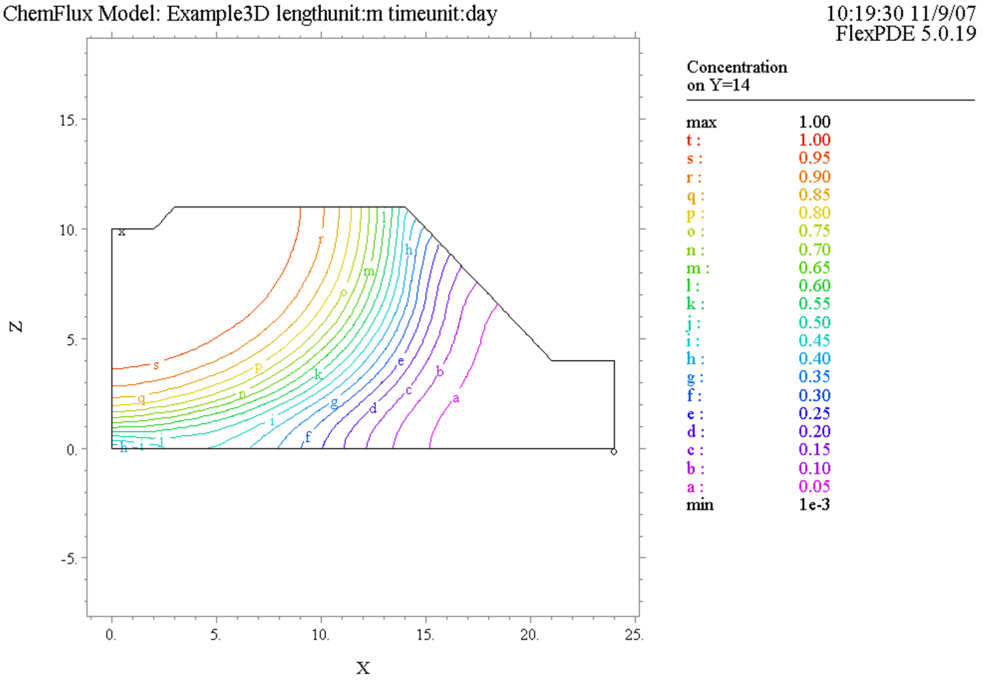
1. *Open ACUMESH: View* > *ACUMESH* menu option
2. *Plot Contours: Plot* > *Contours*
3. *Model State: States* toolbar drop-down

1.4.1.2 Results and Discussion

After the model has finished solving, the results will be displayed in the dialog of thumbnail plots within the CHEMFLUX solver. Right-click the mouse and select *Maximize* to enlarge any of the thumbnail plots. This section will give a brief analysis for each plot that was generated.

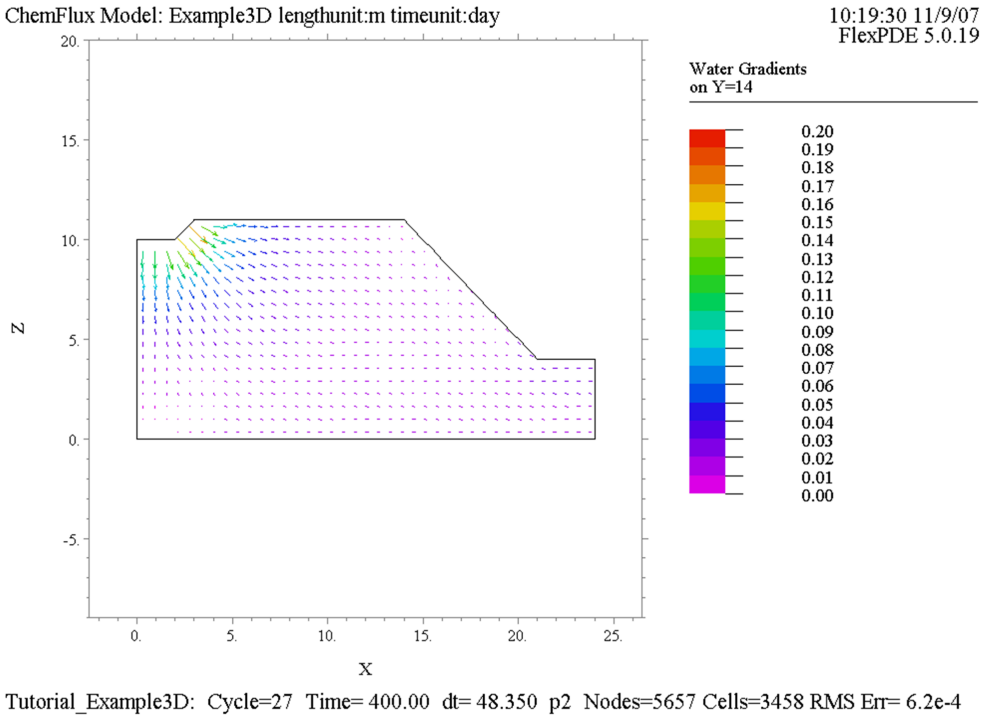


The Mesh plot displays the finite element mesh generated by the solver. The mesh is automatically refined in critical areas. Right-click on the plot and select *Rotate* to enable the rotate window.



Tutorial_Example3D: Cycle=27 Time= 400.00 dt= 48.350 p2 Nodes=5657 Cells=3458 RMS Err= 6.2e-4
Integral= 116.3422

In this contour plot it can be seen the concentration is equal to 1 at the reservoir and decreases to *0* at the river.

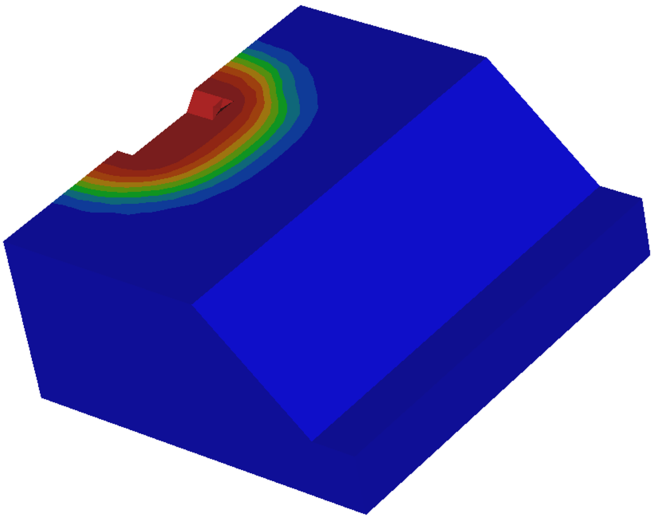


Gradient Vectors show both the direction and the magnitude of the flow at specific points in the model. Vectors illustrate that flow is from right to left towards the river in this view with higher gradients near the reservoir.

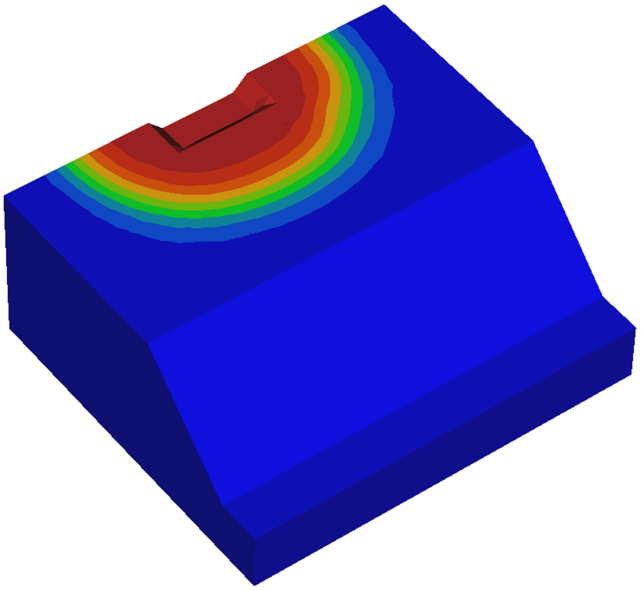
The following is a short summary of plots created in ACUMESH illustrating the movement of the plume through the model for times of 50 days, 100 days, and 400 days. Note that the plume does not reach the river channel in within the 400 day time period. The below diagram was created in ACUMESH by plotting concentration contours and varying time:

1. Open ACUMESH by selecting *Window > ACUMESH* from the menu.
2. Select *Plots > Contours* from the menu.
3. Select *c* from the Variable Name drop-down.
4. Click *OK* to close the Contours dialog.
5. Select the desired timestep from the *Time* drop-down on the toolbar.

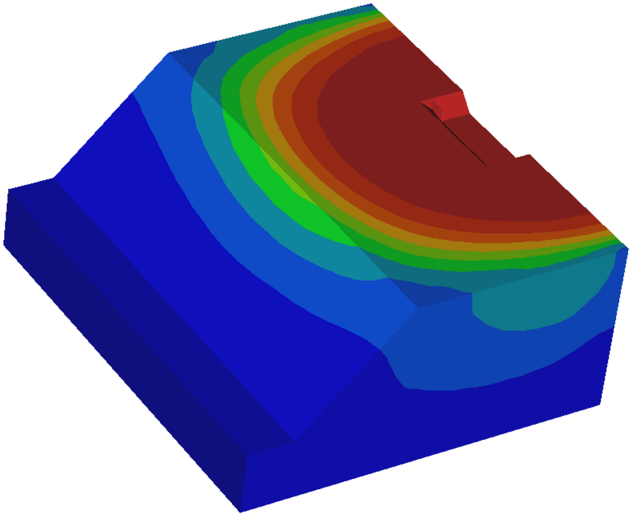
- **Time = 50 days**



- **Time = 100 days**



- **Time = 400 days**



1.4.2 Appendix B

- **Surface 1 Grid**

X	Y	Z		X	Y	Z
0	0	0		14	0	0
0	10	0		14	10	0
0	11	0		14	11	0
0	16	0		14	16	0
0	17	0		14	17	0
0	27	0		14	27	0
2	0	0		21	0	0
2	10	0		21	10	0
2	11	0		21	11	0
2	16	0		21	16	0
2	17	0		21	17	0
2	27	0		21	27	0
3	0	0		24	0	0
3	10	0		24	10	0
3	11	0		24	11	0
3	16	0		24	16	0
3	17	0		24	17	0
3	27	0		24	27	0

- **Surface 2 Grid**

X	Y	Z		X	Y	Z
0	0	11		14	0	11
0	10	11		14	10	11
0	11	10		14	11	11
0	16	10		14	16	11
0	17	11		14	17	11
0	27	11		14	27	11
2	0	11		21	0	4
2	10	11		21	10	4
2	11	10		21	11	4
2	16	10		21	16	4
2	17	11		21	17	4
2	27	11		21	27	4
3	0	11		24	0	4
3	10	11		24	10	4
3	11	11		24	11	4
3	16	11		24	16	4
3	17	11		24	17	4
3	27	11		24	27	4